

## WEST Search History

DATE: Monday, May 10, 2004

**Hide? Set Name Query** **Hit Count**

*DB=PGPB,USPT; PLUR=YES; OP=ADJ*

<input type="checkbox"/>	L12	l11 and catechol	0
<input type="checkbox"/>	L11	l6 and l10	6
<input type="checkbox"/>	L10	polymerization inhibitor	8729
<input type="checkbox"/>	L9	l6 and l8	1
<input type="checkbox"/>	L8	cyclohexanecarbonyl chloride	463
<input type="checkbox"/>	L7	cyclohexanevarbonyl chloride	0
<input type="checkbox"/>	L6	l5 and (chlorinat\$ or halogenat\$)	30
<input type="checkbox"/>	L5	l4 and hydrogenat\$	37
<input type="checkbox"/>	L4	l3 and carboxylic acid	93
<input type="checkbox"/>	L3	l2 and acrylic acid	139
<input type="checkbox"/>	L2	l1 and \$butadiene	176
<input type="checkbox"/>	L1	cyclohexyl phenyl ketone	539

END OF SEARCH HISTORY

## WEST Search History

DATE: Monday, May 10, 2004

**Hide? Set Name Query** **Hit Count**

*DB=PGPB,USPT; PLUR=YES; OP=ADJ*

<input type="checkbox"/>	L3	l2 and acrylic acid	0
<input type="checkbox"/>	L2	l1 and butadiene	11
<input type="checkbox"/>	L1	cycloalkyl aryl ketone\$	17

END OF SEARCH HISTORY

=> d his

(FILE 'HOME' ENTERED AT 22:52:08 ON 10 MAY 2004)

FILE 'CASREACT' ENTERED AT 22:52:27 ON 10 MAY 2004

L1                   STRUCTURE UPLOADED  
L2                   0 S L1  
L3                   25 S L1 FULL

FILE 'CAPLUS' ENTERED AT 22:53:40 ON 10 MAY 2004

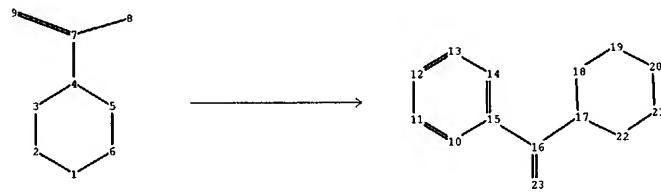
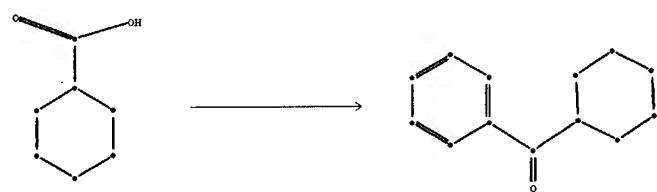
L4                   5256 S ?PHENYL KETONE?  
L5                   1033 S L4 AND CYCLOHEX?  
L6                   76 S L5 AND ?DIENE  
L7                   5 S L6 AND ACRYLIC ACID  
L8                   204 S L4 AND ?DIENE  
L9                   13 S L8 AND ACRYLIC ACID  
L10                  20 S L4 AND DIELS-ALDER?  
L11                  2 S L10 AND ?CARBOXYLIC ACID  
L12                  372 S L4 AND ?CARBOXYLIC ACID  
L13                  16 S L12 AND (HALOGENAT? OR CHLORINAT?)  
L14                  3 S L13 AND HYDROGENAT?  
L15                  170 S L12 AND ?CHLORIDE  
L16                  4994 S POLYMERIZATION INHIBITOR?  
L17                  385 S L16 AND ?CATECHOL  
L18                  0 S L12 AND L17  
L19                  2 S L8 AND ?CATECHOL  
L20                  1 S L13 AND ?CATECHOL  
L21                  2 S L6 AND ?CATECHOL

L14 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 2004:307622 CAPLUS  
DOCUMENT NUMBER: 140:303405  
TITLE: Preparation of cyclohexyl **phenyl**  
**ketone** from 1,3-butadiene and acrylic acid  
without purification of intermediates  
INVENTOR(S): Ju, Yeong-je; Kim, Jin-eok; Won, Jeong-im; Kan, Tae-yi  
PATENT ASSIGNEE(S): Korea Kumho Petrochemical Co., Ltd., S. Korea  
SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.  
CODEN: JKXXAF  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004115499	A2	20040415	JP 2003-201414	20030724
US 2004073068	A1	20040415	US 2003-628800	20030728

PRIORITY APPLN. INFO.: KR 2002-58627 A 20020927

AB Cyclohexyl Ph ketone, useful as an intermediate for photoinitiator 1-hydroxycyclohexyl Ph ketone (no data), is prepared by [2+4] Diels-Alder reaction of 1,3-butadiene with acrylic acid in the presence or absence of solvents, **hydrogenation** of 3-cyclohexene-1-**carboxylic acid**, without purification, **chlorination** of the resulting **cyclohexanecarboxylic acid** solution, and without separation of intermediate chloride and byproducts, Friedel-Crafts reaction of the chloride in the same reactor. Acrylic acid was reacted with 1,3-butadiene in the presence of 4-tert-butylcatechol in benzene at 120° for 2 h, **hydrogenated** using Pd/C under 120 psi H at 100°, and **chlorinated** with SOCl<sub>2</sub> in benzene under reflux for 1 h to give cyclohexanecarbonyl chloride, which was treated with AlCl<sub>3</sub> under reflux for 1 h to give cyclohexyl Ph ketone with ≥99% selectivity at 99% conversion.



chain nodes :

7 8 9 16 23

ring nodes :

1 2 3 4 5 6 10 11 12 13 14 15 17 18 19 20 21 22

chain bonds :

4-7 7-8 7-9 15-16 16-17 16-23

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 10-11 10-15 11-12 12-13 13-14 14-15  
17-18 17-22 18-19 19-20 20-21 21-22

exact/norm bonds :

16-23

exact bonds :

1-2 1-6 2-3 3-4 4-5 4-7 5-6 15-16 16-17 17-18 17-22 18-19  
19-20 20-21 21-22

normalized bonds :

7-8 7-9 10-11 10-15 11-12 12-13 13-14 14-15

isolated ring systems :

containing 1 : 10 : 17 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS  
10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:Atom  
18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:CLASS

fragments assigned product role:

containing 10

fragments assigned reactant/reagent role:

containing 1

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

Structure attributes must be viewed using STN Express query preparation.

=> s 11

SAMPLE SEARCH INITIATED 22:52:49 FILE 'CASREACT'

SCREENING COMPLETE - 31 REACTIONS TO VERIFY FROM

5 DOCUMENTS

100.0% DONE 31 VERIFIED 0 HIT RXNS 0 DOCS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*

PROJECTED VERIFICATIONS: 286 TO 954

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1 ( 0 REACTIONS)

=> s 11 full

FULL SEARCH INITIATED 22:52:54 FILE 'CASREACT'

SCREENING COMPLETE - 600 REACTIONS TO VERIFY FROM 105 DOCUMENTS

100.0% DONE 600 VERIFIED 60 HIT RXNS 25 DOCS  
SEARCH TIME: 00.00.01

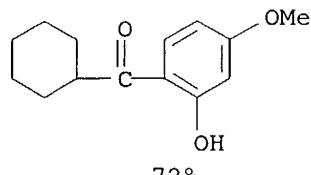
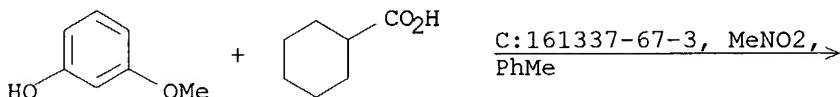
L3 25 SEA SSS FUL L1 ( 60 REACTIONS)

=> d scan

L3 25 ANSWERS CASREACT COPYRIGHT 2004 ACS on STN

TI Catalytic direct C-acylation of phenol and naphthol derivatives using carboxylic acids as acylating reagents

RX(4) OF 4



NOTE: regioselective

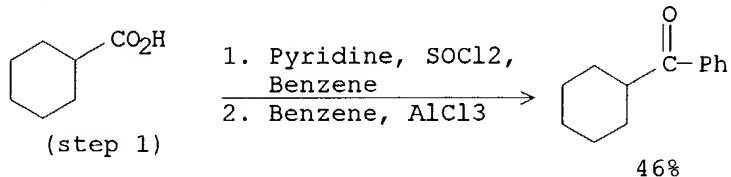
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):5

L3 25 ANSWERS CASREACT COPYRIGHT 2004 ACS on STN

TI Synthesis and structure-activity relationships of potential

anticonvulsants based on 2-piperidinecarboxylic acid and related pharmacophores

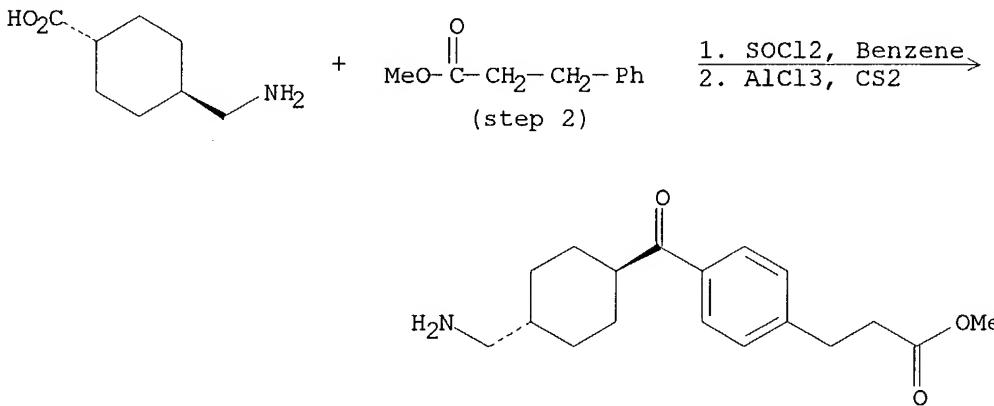
RX(2) OF 193



L3 25 ANSWERS CASREACT COPYRIGHT 2004 ACS on STN

TI A facile synthesis of aminocarboxylic acid derivatives, new anti-ulcer agents

RX(8) OF 13 - 2 STEPS

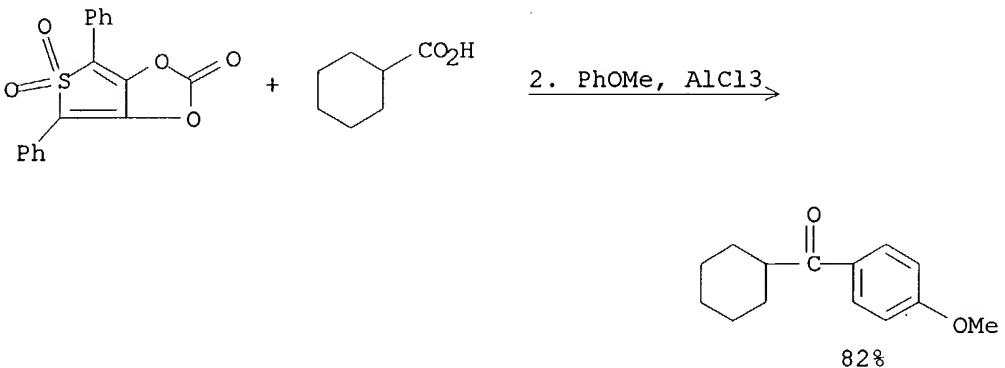


HCl

L3 25 ANSWERS CASREACT COPYRIGHT 2004 ACS on STN

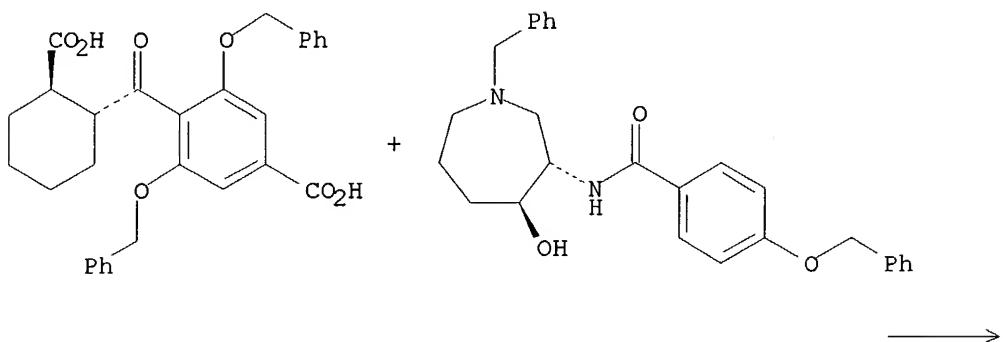
TI 4-Acyloxy-2,5-diphenyl-3-oxo-2,3-dihydrothiophene 1,1-dioxides as acylating agents in the Friedel-Crafts reaction

RX(35) OF 47 - 2 STEPS

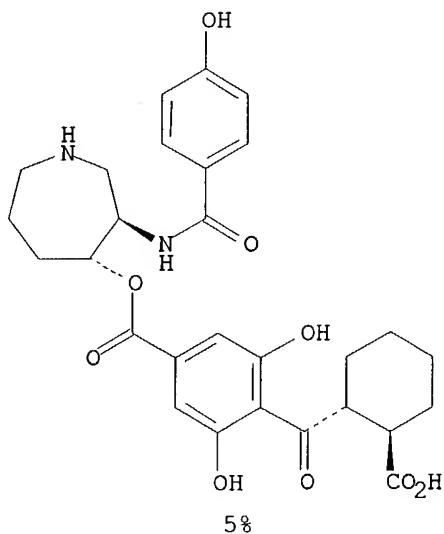


TI Synthesis and Protein Kinase Inhibitory Activity of Balanol Analogue with Modified Benzophenone Subunits

RX(77) OF 305



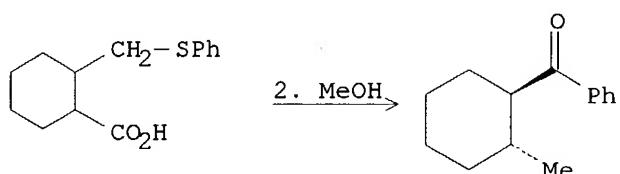
RX(77) OF 305

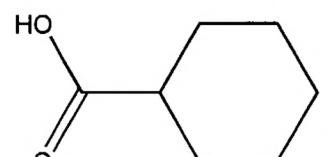


NOTE: general procedure available

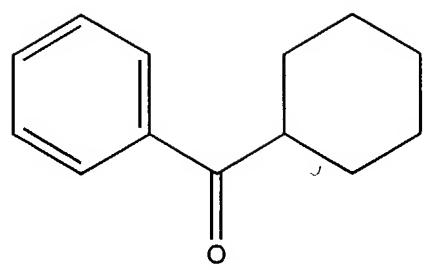
TI Syntheses of 6,6a,7,8,9,10,10a,11-octahydro-11-oxodibenz[b,e]oxepins and 6,6a,7,8,9,10,10a,11-octahydro-11-oxodibenzo[b,e]thiepins

RX(11) OF 14 - 2 STEPS





cyclohexanecarboxylic acid



cyclohexyl phenyl ketone